Molecular Biology

A MATHEMATICAL MODEL OF CAPSULAR EXOPOLYSACCHARIDE SYNTHESIS IN *ESCHERICHIA COLI*, <u>Kimberly A. Spotts¹</u>, S.M. Baer²*, and V. Stout¹*, Arizona State University, Departments of Microbiology¹ and Mathematics², Tempe, AZ 85287, kspotts@imap2.asu.edu.

The colanic acid biosynthesis pathway in *Escherichia coli* is of both scientific and medical importance because it may be responsible for many antibiotic resistant infections due to biofilm formation. However, it is often difficult to experimentally demonstrate the mechanisms of the regulation of this system, so a mathematical model was developed which can be compared to experimental data obtained in the laboratory. Using the Law of Mass Action, which allows one to compose a set of differential equations which describe a particular biochemical system, one hundred seven differential equations were developed. Also, several experiments were completed in order to calibrate the rate constants and several of the parameters from the model. When modeled on a computer, these equations give some idea of the ways in which the expression of the capsular polysaccharide synthesis (cps) operon in E. coli is affected by several regulatory molecules in the pathway. The output from these equations has successfully been compared to experimental data already collected on the system in order to mimic the mechanisms of capsule biosynthesis and reveal data concerning the kinetics of capsule expression. The output also creates an image of the kinetics behind the two-component regulatory system which controls expression of the cps operon. It is expected that in the future the model may provide the basis for new experimentation on the pathway. This mathematical model has made it possible to start generating hypotheses about biochemical interactions which could not efficiently be studied in most cases. These equations are expected to be the starting ground for the elucidation of several unanswered questions about colanic acid synthesis in E. coli, making cures for antibiotic resistant infections more readily attainable.

Methods